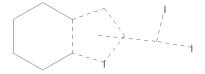
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ring nodes :

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chain bonds :
10-12 10-11
ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 10-12 \quad 10-11$ 

isolated ring systems :

containing 1:

Match level :

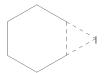
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ring nodes :

1 2 3 4 5 6 7

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-7

exact/norm bonds :

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isolated ring systems :

containing 1 :

Match level :

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L4 STRUCTURE UPLOADED

L1 STRUCTURE UPLOADED

L2 50 S L1

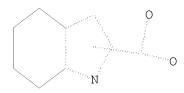
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L1 STR



Structure attributes must be viewed using STN Express query preparation.

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Structure attributes must be viewed using STN Express query preparation.

L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:523418 CAPLUS <<LOGINID::20080502>>

DN 143:44076

TI A method for the preparation of (2S,3aR,7aS)-octahydro-1H-indole-2-carboxylic acid as key intermediate in the preparation of trandolapril by reacting a cyclohexyl aziridine with a dialkyl malonate

IN Cid, Pau

PA Texcontor Etablissement, Liechtenstein

SO PCT Int. Appl., 34 pp. CODEN: PIXXD2

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DT
    Patent
LA
    English
FAN.CNT 1
                                     APPLICATION NO.
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PRAI EP 2003-257417
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    WO 2004-EP13377
                              20041125
    CASREACT 143:44076; MARPAT 143:44076
OS
AΒ
    Trandolapril intermediate (2S, 3aR, 7aS)-octahydro-1H-indole-2-carboxylic
    acid (or its C-protected derivs. or salts) was prepared by reacting a
    cyclohexyl aziridine with a dialkyl malonate to form a trans-fused
    3-(alkylcarbonyl)octahydroindol-2-one, decarbonylation at the 3-position,
    conversion of 2-oxo group to an optionally protected carboxylic acid
    group, and removal of any N-substitution. Examples illustrate the
    synthetic method, starting with reaction of cyclohexene with chloramine-T
    to form N-tosylcyclohexanoaziridine.
             THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L12 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
    ΑN
DN
    143:7555
ΤI
    Reactions of Indole Derivatives with Oxiranes and Aziridines on Silica.
    Synthesis of \beta-Carbolin-1-one Mimic of Pancratistatin
ΑU
    Hudlicky, Tomas; Rinner, Uwe; Finn, Kevin J.; Ghiviriga, Ion
CS
    Department of Chemistry, Brock University, St. Catharines, ON, L2S 3A1,
    Can.
    Journal of Organic Chemistry (2005), 70(9), 3490-3499
SO
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CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society

CASREACT 143:7555

PΒ

DT

LA

OS GI Journal

English

Ι

AB Indole and several indoles functionalized at C-2 were condensed with oxiranes, vinyloxiranes, aziridines, and vinylaziridines in the solid state on the surface of silica. The yields of these reactions were compared to those obtained from Lewis acid-catalyzed ring-opening reactions performed in solution and found to be superior in each case. The solid state aziridine opening constituted a key step in the synthesis of the  $\beta$ -carbolin-1-one mimic of pancratistatin. Me 2-indolecarboxylate was found to react on the silica gel surface with N-tosylvinylaziridine in 68% yield. A nine-step synthesis of the pancratistatin mimic I has been attained. The addnl. key transformation in this synthesis involved silica gel-catalyzed opening of an epoxide and hydrolysis of an acetonide. Detailed exptl. procedures and full characterization are reported for all new compds.

IT 1202-04-6 68820-12-2

RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of  $\beta$ -carbolin-1-one mimic of pancratistatin via reactions of indole derivs. with oxiranes and aziridines in the solid state on the surface of silica)

RN 1202-04-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, methyl ester (CA INDEX NAME)

RN 68820-12-2 CAPLUS

CN 7-Azabicyclo[4.1.0]heptane, 7-[(4-methylphenyl)sulfonyl]- (CA INDEX NAME)

IT 811419-63-3P 811419-64-4P 811419-67-7P

811419-68-8P 811419-71-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(synthesis of  $\beta$ -carbolin-1-one mimic of pancratistatin via reactions of indole derivs. with oxiranes and aziridines in the solid state on the surface of silica)

RN 811419-63-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[(3aS,4R,5R,7aR)-3a,4,5,7a-tetrahydro-2,2-dimethyl-4-[[(4-methylphenyl)sulfonyl]amino]-1,3-benzodioxol-5-yl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

RN 811419-64-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[(3aS,4R,5R,7aR)-3a,4,5,7a-tetrahydro-2,2-dimethyl-4-[[(4-methylphenyl)sulfonyl]amino]-1,3-benzodioxol-5-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 811419-67-7 CAPLUS

CN D-epi-Inositol, 3,4-anhydro-5,6-dideoxy-5-[2-(methoxycarbonyl)-1H-indol-3-yl]-1,2-O-(1-methylethylidene)-6-[[(4-methylphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 2-A

RN 811419-68-8 CAPLUS

CN D-epi-Inositol, 3,4-anhydro-5,6-dideoxy-5-[1-[(1,1-dimethylethoxy)carbonyl]-2-(methoxycarbonyl)-1H-indol-3-yl]-6-[[(1,1-dimethylethoxy)carbonyl][(4-methylphenyl)sulfonyl]amino]-1,2-0-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 811419-71-3 CAPLUS

CN D-epi-Inositol, 3,4-anhydro-5,6-dideoxy-6-[[(1,1-dimethylethoxy)carbonyl]-2-(methoxycarbonyl)-1H-indol-3-yl]-1,2-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RE.CNT 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:80349 CAPLUS <<LOGINID::20080502>>

DN 140:146136

Preparation of chemokine receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders

IN Bridger, Gary; Kaller, Al; Harwig, Curtis; Skerlj, Renato; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan,

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Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher D.; Di Fluri,
     Maria R.
PΑ
     USA
     U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of U.S. Ser. No. 446,170.
SO
     CODEN: USXXCO
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     English
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R4

The invention relates to heterocyclic compds. (shown as I; e.g. AΒ (1H-benzimidazol-2-ylmethyl) (piperidin-3-ylmethyl) (5,6,7,8tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. compds. bind to chemokine receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5  $\mu\text{M}$  for inhibition of SDF-1 $\alpha$  induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. It is also stated that the compds. I behave in a manner similar to 1,1'-[1,4-phenylene-bis(methylene)]-bis-1,4,8,11-tetraazacyclotetradecane (AMD3100) which showed to elevate progenitor cell levels (data given). Although the methods of preparation are not claimed, >170 example prepns. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 +one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

RN 1477-50-5 CAPLUS

CN 1H-Indole-2-carboxylic acid (CA INDEX NAME)

IT 298680-75-8P, N-(2-Nitrobenzenesulfonyl)-7azabicyclo[4.1.0]heptane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of chemokine receptor binding benzimidazolylmethyl tetrahydroquinolinyl amines and related heterocyclic compds. with enhanced efficacy against AIDS and other disorders)

RN 298680-75-8 CAPLUS

CN 7-Azabicyclo[4.1.0]heptane, 7-[(2-nitrophenyl)sulfonyl]- (CA INDEX NAME)

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L12 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
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AN 2003:532661 CAPLUS <<LOGINID::20080502>>

DN 139:101128

TI Preparation of chemokine receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders

IN Bridger, Gary J.; Skerlj, Renato T.; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di Fluri, Rosaria Maria

PA Anormed Inc., Can.; et al.; et al.

SO PCT Int. Appl., 360 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

GΙ

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AΒ The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. compds. bind to chemokine receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5  $\mu\text{M}$  for inhibition of SDF-1 $\alpha$  induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. Although the methods of preparation are not claimed, >170 example prepns. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 =  $\geq$  2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + anotherR5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

IT 1477-50-5, Indole-2-carboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chemokine receptor binding benzimidazolylmethyl tetrahydroquinolinyl amines and related heterocyclic compds. with enhanced efficacy against AIDS and other disorders)

RN 1477-50-5 CAPLUS

CN 1H-Indole-2-carboxylic acid (CA INDEX NAME)

IT 298680-75-8P, N-(2-Nitrobenzenesulfonyl)-7 azabicyclo[4.1.0]heptane
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of chemokine receptor binding benzimidazolylmethyl)

tetrahydroquinolinyl amines and related heterocyclic compds. with enhanced efficacy against AIDS and other disorders)

RN 298680-75-8 CAPLUS

CN 7-Azabicyclo[4.1.0]heptane, 7-[(2-nitrophenyl)sulfonyl]- (CA INDEX NAME)

## RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:881494 CAPLUS <<LOGINID::20080502>>

DN 139:214244

TI Product class 5: 1H-azirines

AU Zeller, K.-P.

CS Institut fuer Organische Chemie, Universitaet Tuebingen, Tuebingen, 72076, Germany

SO Science of Synthesis (2002), 9, 67-83 CODEN: SSCYJ9

PB Georg Thieme Verlag

DT Journal; General Review

LA English

AB A review discusses the role of 1H-azirines as short-lived reaction intermediates and their isolation and characterization by spectroscopic techniques in low-temperature matrixes. The reaction of alkynes with nitrenes or nitrene equivalent and the generation of nitrene (NH) from hydrazoic acid are described.

IT 942-24-5P, 3-Methoxycarbonylindole 1202-04-6P, 2-Methoxycarbonylindole

RL: SPN (Synthetic preparation); PREP (Preparation)

(azirines as intermediates in dinitrogen elimination of triazoles)

RN 942-24-5 CAPLUS

CN 1H-Indole-3-carboxylic acid, methyl ester (CA INDEX NAME)

RN 1202-04-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, methyl ester (CA INDEX NAME)

IT 6574-00-1, 7-Azabicyclo[4.1.0]hepta-1,3,5-triene RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (generation of cyclic  $\alpha$ -imino carbenes from benzotriazoles with formation of transient benzo[b]azirine)

RN 6574-00-1 CAPLUS

CN 7-Azabicyclo[4.1.0]hepta-1,3,5-triene (CA INDEX NAME)



RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1975:531405 CAPLUS <<LOGINID::20080502>>

DN 83:131405

OREF 83:20665a,20668a

TI Aminoethylation. II. Reactions of meso-cis-cyclohexenimine and its derivative with diethyl malonate. Synthesis of trans-octahydroindole

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SO Yakugaku Zasshi (1975), 95(7), 889-92 CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Japanese

OS CASREACT 83:131405

GI For diagram(s), see printed CA Issue.

AB Meso-cis-cyclohexenimine or N-benzylsulfonyl-meso-cis-cyclohexenimine reacted with sodium ethyl malonate in EtOH or (EtO)2CO to give 2-oxo-3-ethoxycarbonyl-trans-octahydroindole or N-benzylsulfonyl-2-oxo-3-ethoxycarbonyl-trans-octahydroindole I (R = H, PhCH2SO2, resp.). Reduction of octahydro-2-oxoindole, which was obtained after hydrolysis and decarboxylation of I (R = H) with LiAlH4 gave trans-octahydroindole.

IT 56921-06-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and decarboxylation of)

RN 56921-06-3 CAPLUS

CN 1H-Indole-3-carboxylic acid, octahydro-2-oxo- (CA INDEX NAME)

IT 56921-03-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 56921-03-0 CAPLUS

CN 1H-Indole-3-carboxylic acid, octahydro-2-oxo-, ethyl ester (CA INDEX NAME)

IT 56251-85-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with malonate, indole derivative from)

RN 56251-85-5 CAPLUS

CN 7-Azabicyclo[4.1.0]heptane, 7-[(phenylmethyl)sulfonyl]- (CA INDEX NAME)

$$Ph-CH_2-S-N$$

IT 56921-04-1P 56921-05-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 56921-04-1 CAPLUS

CN Propanoic acid,  $3-[[2-(7-azabicyclo[4.1.0]hept-7-y1)cyclohexyl]amino]-3-oxo-, ethyl ester, <math>[1\alpha, 6\alpha, 7(1R^*, 2R^*)]-(9CI)$  (CA INDEX NAME)

Relative stereochemistry.

RN 56921-05-2 CAPLUS

CN 1H-Indole-3-carboxylic acid, octahydro-2-oxo-1-[(phenylmethyl)sulfonyl]-, ethyl ester (CA INDEX NAME)

1]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN 1972:461723 CAPLUS <<LOGINID::20080502>> DN 77:61723 OREF 77:10207a,10210a ΤI Synthesis and reactions of 3-indolyl  $\beta$  ketones ΑU CS Pharm.-Res. Canada Ltd., Pointe Claire, QC, Can. SO Journal of Organic Chemistry (1972), 37(12), 2010-15 CODEN: JOCEAH; ISSN: 0022-3263 DTJournal LA English GΙ For diagram(s), see printed CA Issue. AB Reaction of indoles with free 3 position with  $\alpha\text{-halo}$  ketones in acidic solns. affords 3-indolyl ketones. This novel reaction conveniently offers versatile starting materials for indolyl-cyclohexyl oximes (e.g., I), amines, alcs., indolyl-azabicycloheptanes (e.g., II), and indolylfatty acids, as well as pyrano[3,4-b]indoles (e.g., III). 32500-47-3P 32500-54-2P 32500-55-3P ΙT 32544-47-1P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 32500-47-3 CAPLUS RN 1H-Indole-2-carboxylic acid, 3-[2-[(aminothioxomethyl))hydrazono]cyclopenty

RN 32500-54-2 CAPLUS CN 7-Azabicyclo[4.1.0]heptane, 2-(1,2-dimethyl-1H-indol-3-yl)-,  $(1\alpha,2\beta,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 32500-55-3 CAPLUS CN 7-Azabicyclo[4.1.0]heptane, 2-(1,2-dimethyl-1H-indol-3-yl)-,  $(1\alpha,2\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 32544-47-1 CAPLUS CN 1H-Indole-2-carboxylic acid, 1-methyl-3-(2-oxocyclopentyl)-, ethyl ester (CA INDEX NAME)